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Simple theory of extremely overdoped HTS

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Abstract

We demonstrate the existence of a simple physical picture of superconductivity for extremely overdoped CuO_2 planes. It possesses all characteristic features of HTS, such as a high superconducting transition temperature, the $d_{x^2-y^2}$ symmetry of order parameter, and the coexistence of a single electron Fermi surface and a pseudogap in the normal state. Values of pseudogap are calculated for different doping levels. An orbital paramagnetism of preformed pairs is predicted.

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1 Introduction

In this work (see also earlier Letter [1]), we demonstrate that, in the phase diagram of cuprate HTS, a small region exists in which the characteristic features of HTS can be easily understood on the bases of a simple theory. The above characteristic features are such as a high superconducting transition temperature, the $d_{x^2-y^2}$ symmetry of order parameter (see [2]), and the coexistence in the normal state of a single electron Fermi surface and a pseudogap [3]. The latter phenomenon is usually attributed to the presence of preformed (*i.e.*, in the normal state) electron pairs (in particular, bipolarons [4-8]).

The aforementioned small region in the phase diagram is situated in the vicinity of the maximal hole-doping level $x = x_c$ compatible with superconductivity. The superconducting transition temperature T_c is zero for $x \geq x_c$, so it is low in our region near $x = x_c$. However, T_c increases with decreasing x for $x < x_c$ in such a way that at the boundary of the region (i.e., for $x_c - x \sim 1$) it is quite high.

Two features of our small region are important to make a simple physical picture possible. These are relatively low T_c and the clear nature of the normal state as mostly the conventional Fermi liquid.

We calculate the pseudogap. With increasing x, the pseudogap decreases for $x < x_c$. As well as T_c, the pseudogap disappears at $x = x_c$. However, for larger doping levels $x > x_c$, it appears again.

As a new prediction, we show the existence of an unusual orbital paramagnetism of the preformed (singlet) pairs, which probably can be experimentally separated from the Pauli spin paramagnetism of single electrons and the Landau diamagnetism of single electrons and pairs.

2 Pair quasiparticles

The key point is the existence of very mobile pair quasiparticles in crystals in conditions of the tight-binding, *i.e.*, if the energy of electron-electron interaction at a distance on the order of atomic spacing considerably exceeds the electron-tunneling amplitude to neighboring lattice cites. Quasiparticles of this type were studied earlier [9] in helium quantum crystals and more recently by Alexandrov and Kornilovitch [7] as a model of bipolarons in HTS (see also [10]).

Let us consider two electrons localized at neighboring (1 and 2 in the figure) copper atoms (to be more precise, in unit cells containing these atoms) forming a square lattice in the CuO_2 plane. The electron tunneling from 2 to 4 or 6 does not change the energy of the system in view of the crystal lattice symmetry. The same is true for the electron tunneling from 1 to 3 or 5. Owing to this type of transitions, an electron

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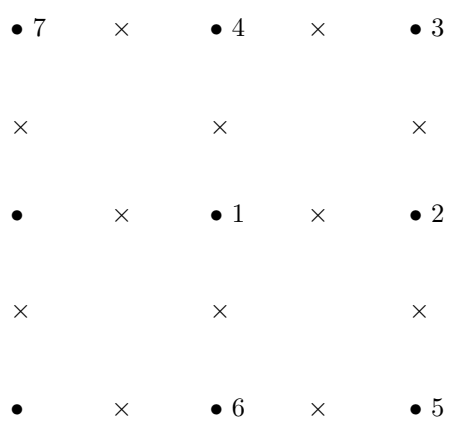

Figure 1: CuO_2 plane: (•) Cu atoms and (×) O atoms.

pair can move as a whole over the entire plane, since the $2 \to 4$ transition can be followed by the transition $1 \to 7$ or $1 \to 3$, and so on. Since the transitions do not change the energy of the system, the motion is fully coherent. An electron pair behaves as a delocalized Bose quasiparticle.

To calculate the quasiparticle spectrum, we consider the localized states of a pair,

$$|\mathbf{r}, \mathbf{r}', \alpha\beta\rangle = c^+_{\mathbf{r}\alpha} c^+_{\mathbf{r}'\beta} |0\rangle , \tag{1}$$

where $c^+_{\mathbf{r}\alpha}$ are the electron creation operators at point $\mathbf{r}$ with spin projection $\alpha = \uparrow, \downarrow$ and $|0\rangle$ is the electron vacuum.

The effective tunneling Hamiltonian H_{eff} is defined by the matrix elements of the operator

$$H = t \sum_{\mathbf{r}\mathbf{r}'\alpha} c^+_{\mathbf{r}'\alpha} c_{\mathbf{r}\alpha}, \tag{2}$$

which correspond to the transitions of one of the electrons to copper atoms that are next-to-nearest neighbors of the initial atom, in such a way that the energy of the system of two electrons remains unchanged. Here, t is the tunneling amplitude, which is known to be positive (see [2], p. 1004).

Let $\mathbf{a}_n$ $(n = x, y)$ be the square-lattice periods directed from point 1 to point 2 and from point 1 to point 4, respectively. We have

$$\begin{aligned} H_{eff} |\mathbf{r}, \mathbf{r} + \mathbf{a}_x, \alpha\beta\rangle = t(|\mathbf{r} + \mathbf{a}_x + \mathbf{a}_y, \mathbf{r} + \mathbf{a}_x, \alpha\beta\rangle + |\mathbf{r} + \mathbf{a}_x - \mathbf{a}_y, \mathbf{r} + \mathbf{a}_x, \alpha\beta\rangle + \\ |\mathbf{r}, \mathbf{r} + \mathbf{a}_y, \alpha\beta\rangle + |\mathbf{r}, \mathbf{r} - \mathbf{a}_y, \alpha\beta\rangle) = t(- |\mathbf{r} + \mathbf{a}_x, \mathbf{r} + \mathbf{a}_x + \mathbf{a}_y, \beta\alpha\rangle + |\mathbf{r} + \mathbf{a}_x - \mathbf{a}_y, \mathbf{r} + \mathbf{a}_x, \alpha\beta\rangle + \\ |\mathbf{r}, \mathbf{r} + \mathbf{a}_y, \alpha\beta\rangle - |\mathbf{r} - \mathbf{a}_y, \mathbf{r}, \beta\alpha\rangle), \end{aligned} \tag{3}$$

where we used the antisymmetry of quantities (1) with respect to arguments $(\mathbf{r}, \alpha)$ and $(\mathbf{r}', \beta)$. Analogously,

$$\begin{aligned} H_{eff} |\mathbf{r}, \mathbf{r} + \mathbf{a}_y, \alpha\beta\rangle = t(- |\mathbf{r} + \mathbf{a}_y, \mathbf{r} + \mathbf{a}_x + \mathbf{a}_y, \beta\alpha\rangle + |\mathbf{r} - \mathbf{a}_x + \mathbf{a}_y, \mathbf{r} + \mathbf{a}_y, \alpha\beta\rangle + \\ |\mathbf{r}, \mathbf{r} + \mathbf{a}_x, \alpha\beta\rangle - |\mathbf{r} - \mathbf{a}_x, \mathbf{r}, \beta\alpha\rangle). \end{aligned} \tag{4}$$

The complete set of localized states of an electron pair is determined by the state vectors

$$|\mathbf{r}, n, \alpha\beta\rangle \equiv |\mathbf{r}, \mathbf{r} + \mathbf{a}_n, \alpha\beta\rangle , \tag{5}$$

where $\mathbf{r}$ labels unit cells of the square lattice.

The problem obviously splits into two independent problems for singlet and triplet pairs that are characterized by quantities (5), respectively, antisymmetric and symmetric about the spin indices α, β. Assuming that the required stationary states of a pair are superpositions of localized states,

$$\sum_{\mathbf{r}, n} \psi^{(n)}_{\alpha\beta} e^{i\mathbf{k}\mathbf{r}} |\mathbf{r}, n, \alpha\beta\rangle \tag{6}$$

with coefficients $\psi_{\alpha\beta}^{(n)}$ independent of $\mathbf{r}$ (this corresponds to a definite quasimomentum $\mathbf{k}$), we obtain

$$(E(\mathbf{k}) - \epsilon_0)\psi^{(x)} = t\psi^{(y)}(1 \pm e^{-i\kappa_x})(1 \pm e^{i\kappa_y}),$$
$$(E(\mathbf{k}) - \epsilon_0)\psi^{(y)} = t\psi^{(x)}(1 \pm e^{i\kappa_x})(1 \pm e^{-i\kappa_y}), \quad (7)$$

where the upper or lower sign corresponds to a singlet or triplet state, respectively. The conditions for the existence of a nontrivial solution $\psi^{(x)}$, $\psi^{(y)}$ to system (7) defines the energy $E(\mathbf{k})$ of a pair quasiparticle. Here ϵ_0 is the energy of the initial localized state; $\kappa_x = \mathbf{k}\mathbf{a}_x$ and $\kappa_y = \mathbf{k}\mathbf{a}_y$. Everywhere in formulas (7), we omitted identical spin indices $\alpha\beta$.

The minimal energy $\epsilon_m = \min E(\mathbf{k}) = \epsilon_0 - 4t$ of a singlet pair is attained for $\kappa_x = \kappa_y = 0$. The same minimal energy of a triplet pair is attained for a nonzero quasimomentum $\kappa_x = \kappa_y = \pi$. This degeneracy is removed by taking into account the electron exchange in the initial localized pair. It is well known that this exchange is of an antiferromagnetic nature and, hence, singlet pairs possess the minimal energy.

Thus, solitary Bose quasiparticles can exist in the CuO_2 plane; these particles are characterized by a doubled electric charge and by zero momentum and spin in the ground state. It can readily be seen from Eqs. (7) that the effective mass of quasiparticles is $m = \hbar^2/ta^2$, where $a = |\mathbf{a}_x| = |\mathbf{a}_y|$. In addition, quasiparticles possess a specific quantum number $n = x, y$, which determines the orientation of a two-electron "dumbbell". Substituting $E(\mathbf{k}) = \epsilon_m$ and $\mathbf{k} = 0$ into Eqs. (7), we obtain $\psi^{(x)} = -\psi^{(y)}$ in the ground state. Since orientations $n = x$ and $n = y$ are transformed into each other upon the lattice rotation through an angle of $\pi/2$ and upon the reflection in the diagonal plane passing through points 1 and 3 in the figure, the ground-state wave function $\psi \equiv \psi^{(x)} = -\psi^{(y)}$ of quasiparticles transforms in accordance with the nontrivial 1D representation (usually denoted by $d_{x^2-y^2}$) of the symmetry group of CuO_2 plane (see [2]).

3 Superconductivity

We further assume that all other two-, three-, etc., electron configurations localized at distances on the order of atomic spacing are energetically disadvantageous as compared to the pair configuration considered above. In addition, we assume that electrons are repulsed at large distances such that the electron-electron interaction energy is on the order of the one-electron tunneling amplitude. Under these conditions, only single electron Fermi particles and the pair Bose particles considered above play a significant role.

Finally, let us assume that the minimal energy ϵ_m of pair quasiparticles is such that $\epsilon_m/2$ is within a single electron energy band. We note the following. In conditions of the tight-binding, there are two different situations in which $\epsilon_m/2$ can be within a single electron energy band. First, if single electrons and electrons in pairs correspond to the same energy band, single electron tunneling amplitude should be of the order of the electron-electron interaction energy in the pairs, while one-electron tunneling amplitude t in the pairs, introduced in Section 2, should be much smaller than the interaction. The last condition which is the condition of applicability of the procedure used in Section 2, can be result of the large polaron effect in the pairs. In the second situation, single electrons and electrons in pairs correspond to different bands. Both one-electron amplitudes can be of the same order in this case. The analysis carried out by Alexandrov and Kornilovitch in [7] shows that the conditions formulated above are likely to be realistic.

Let us trace the change of the state of the system at $T = 0$ upon an increase in the number of electrons (decrease in the hole-doping level). Until $\epsilon_m/2 > \epsilon_F$, only single electron quasiparticles are present and the system behaves as an ordinary Fermi liquid. The condition $\epsilon_m/2 = \epsilon_F$ determines the minimal hole-doping level compatible with the state of a normal Fermi liquid. Denote by n_c the corresponding electron density n. Upon a further decrease in the hole-doping level, all additional $n - n_c$ electrons will pass into a Bose-Einstein (BE) condensate of pair quasiparticles (we everywhere consider the case of small $n - n_c$ values, for which the concentration of pairs is low and their interaction can be disregarded). The system becomes a superconductor. The superconducting order parameter represents the boson ground-state wave function $\psi \equiv \psi^{(x)}$ normalized by the condition $|\psi|^2 = (n - n_c)/2$; wave function transforms in accordance with the $d_{x^2-y^2}$ representation of the symmetry group of CuO_2 plane.

It is important to note the following. In the system ground state (i.e., for complete filling of all fermion states with an energy smaller than ϵ_F), the uncertainty in the energy of a boson quasiparticle with low excitation energy $\epsilon = k^2/2m$, arising due to its collisions with single electron Landau quasiparticles, is proportional to ϵ^2. As in the conventional theory of Fermi liquid, this is due, first, to the fact that the density of fermions in the vicinity on the order of ϵ near ϵ_F with which the given boson can collide due to energy conservation, is low. Second, the statistical weight of the final states, to which fermionic transitions

are possible, is small. The probability of the boson decay into two fermions per unit time is also small: as suggested in the beginning of this Section, the boson must overcome a significant energy barrier. Thus, the proposed picture of superconductivity in the vicinity of maximal doping level remains valid even in the region of appreciable densities of fermions, where the interaction between bosons and fermions is significant. The critical electron density n_c is determined from the condition that the electron chemical potential is equal to half of the minimal boson energy. In the general case, the latter is a functional of the distribution function for single electron Landau quasiparticles.

In calculating the superconducting transition temperature, the fermion distribution function may be considered as corresponding to $T = 0$, since the temperature corrections (proportional to T^2) to the thermodynamic functions of Fermi liquid are considerably smaller than the corrections included below.

The density of uncondensed bosons at a finite temperature $T < T_c$ is

$$N' = \int \frac{2\pi k dk}{(2\pi\hbar)^2} \frac{1}{e^{\epsilon/T} - 1} = \frac{mT}{2\pi\hbar^2} \log \frac{T}{\tau}. \tag{8}$$

The integral in Eq. (8) diverges at small ϵ, so that it is cut off at $\epsilon \sim \tau$, where τ is a small tunneling amplitude of electrons in the direction perpendicular to the CuO_2 plane.

The excess number $n - n_c$ of electrons in the system is equal to the doubled sum of N' and number N_0 of bosons in the condensate. This leads to the dependence of the superconducting transition temperature on the doping level for small values of $n - n_c$

$$n - n_c = \frac{mT_c}{\pi\hbar^2} \log \frac{T_c}{\tau} \tag{9}$$

and the number of pairs in the condensate

$$N_0 = \frac{n - n_c}{2} \left(1 - \frac{T}{T_c} \frac{\log T/\tau}{\log T_c/\tau} \right), \tag{10}$$

which determines the modulus of order parameter $|\psi|^2 = N_0$ at finite temperatures. The superconducting transition temperature defined by Eq. (9) is quite high. To within the logarithmic term, this temperature is on the order of one-electron tunneling amplitude t at the boundary of the applicability region (i.e., for $n - n_c \sim a^{-2}$). The possibility that the superconducting transition temperature may have such an order of magnitude was pointed out in the aforementioned paper by Alexandrov and Kornilovitch [7].

The interaction of fermions with the BE condensate (effective electron-electron interaction) that is described by the order parameter ψ creates an effective potential $\Delta_{\mathbf{k}}$ acting on fermions as in conventional superconductors:

$$H_{int} = \sum_{\mathbf{k}} (\Delta_{\mathbf{k}} c^+_{\mathbf{k}\uparrow} c^+_{-\mathbf{k}\downarrow} + \text{h.c.}). \tag{11}$$

In view of the symmetry of ψ, we have

$$\Delta_{\mathbf{k}} = V(\hat{k}_x^2 - \hat{k}_y^2)\psi, \tag{12}$$

where $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$ and V is invariant under the symmetry group.

Owing to this interaction, fermions in the superconducting state considered acquire features typical of an ordinary superconductor with the $d_{x^2-y^2}$ symmetry.

4 Normal state thermodynamics. Pseudogap

The total number of pairs for $T < T_c$ is independent of temperature and equal to $(n - n_c)/2$. The electron chemical potential for $T < T_c$ is also temperature independent and equal to $\mu = \mu(n_c) = \epsilon_m(n_c)/2$ where $\epsilon_m = \epsilon_m(n)$ is the pair minimal energy which depends on fermion density, as it is shown above.

For $T > T_c$, the fermion distribution function, as above, corresponds to $T = 0$, but with the temperature dependent chemical potential. The pair energy spectrum is $E = \epsilon_m(\mu) + \epsilon$ where $\epsilon = k^2/2m$. The pair density above T_c is given by

$$N = \int_0^\infty \frac{2\pi k dk}{(2\pi\hbar)^2} \frac{1}{e^{(\epsilon+\zeta)/T} - 1} = \frac{mT}{2\pi\hbar^2} \log \frac{1}{1 - e^{-\zeta/T}}. \tag{13}$$

The parameter ζ ($\zeta \gg \tau$) is defined by

$$\zeta = \frac{\partial \epsilon_m}{\partial \mu}\delta\mu - 2\delta\mu \tag{14}$$

where $\delta\mu = \mu - \mu(n_c)$. With changing temperature, the total electron number conservation gives

$$n - n_c = 2N + \frac{\partial n}{\partial \mu}\delta\mu. \tag{15}$$

From the last equation, we find $\zeta = \zeta(T)$ and then all other quantities.

For $n > n_c$ and not too high temperature $T \ll T_c \log(T_c/\tau)$, the pair density is determined by

$$\frac{N(T) - N(T_c)}{N(T_c)} = \frac{\partial n/\partial \mu}{2(2 - \partial \epsilon_m/\partial \mu)} T e^{-\Delta_p/T} \tag{16}$$

where $N(T_c) = (n - n_c)/2$ and

$$\Delta_p = T_c \log \frac{T_c}{\tau} = \frac{\pi \hbar^2}{m}(n - n_c) \tag{17}$$

is the pseudogap for $n > n_c$. As well as T_c, it is zero at the critical value of the doping level $n = n_c$. For higher doping level $n < n_c$, ($T_c = 0$), we have

$$N(T) = \frac{mT}{2\pi\hbar^2} e^{-\Delta_p'/T} \tag{18}$$

where

$$\Delta_p' = \left(2\frac{\partial \mu}{\partial n} - \frac{\partial \epsilon_m}{\partial n}\right)(n_c - n) \tag{19}$$

is the pseudogap for $n < n_c$. The equation (18) takes place in the low temperature region $T \ll \Delta_p'$. For $n < n_c$, the pseudogap Δ_p' is the gap in the energy spectrum of the pair quasiparticles. For high temperatures $T \gg \Delta_p, \Delta_p'$ (but $T \ll t$), the pair density is a linear function of temperature:

$$N(T) = \frac{z\partial n/\partial \mu}{2(2 - \partial \epsilon_m/\partial \mu)} T \tag{20}$$

where z is the solution of the equation $\lambda z = e^{-z}$ with

$$\lambda = \frac{\pi \hbar^2}{m} \frac{\partial n/\partial \mu}{2 - \partial \epsilon_m/\partial \mu}. \tag{21}$$

The entropy of pairs is determined by the equation

$$S(T) = \frac{m}{2\pi\hbar^2} \int_0^\infty d\epsilon \{(1+f)\log(1+f) - f \log f\} \tag{22}$$

where $f = \left\{e^{(\epsilon+\zeta)/T} - 1\right\}^{-1}$. For $n > n_c$ in the low temperature region $T \ll \Delta_p$, we have

$$\frac{S(T)}{T} - \left(\frac{S}{T}\right)_{T=T_c} = -\frac{m}{2\pi\hbar^2} \frac{\Delta_p}{T} e^{-\Delta_p/T} \tag{23}$$

where

$$\left(\frac{S}{T}\right)_{T=T_c} = \frac{\pi m}{12\hbar^2}. \tag{24}$$

$S(T)$ is almost linear in T, with exponentially small deviations. For $n < n_c$, the pair entropy is exponentially small at low temperatures $T \ll \Delta_p'$:

$$S(T) = \frac{mT}{2\pi\hbar^2} e^{-\Delta_p'/T}. \tag{25}$$

At high temperatures $T \gg \Delta_p, \Delta_p'$, the entropy is

$$S(T) = \frac{m\sigma}{2\pi\hbar^2} T. \tag{26}$$

The temperature independent factor σ is determined by

$$\sigma = \int_z^\infty \frac{x dx}{e^x - 1} - \lambda z^2. \tag{27}$$

The entropy is again a linear function of temperature.

5 Orbital paramagnetism of pairs

In this Section, we show that the orbital motion of electrons inside the pairs cause a peculiar paramagnetism. Let a pair is at rest as a whole. For singlet pairs at $\mathbf{k} = 0$, the Hamiltonian (3),(4) can be written as a 2x2 matrix

$$H = 4t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \equiv 4t\sigma_1, \tag{28}$$

acting to the state vector ψ,

$$\psi = \psi^{(x)} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \psi^{(y)} \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{29}$$

where $\psi^{(n)}$, $n = x, y$, are quantum amplitudes of two orientations of the two-electron dumbbell, and σ_1 is a Pauli matrix.

In the x-state, coordinates of two electrons (with respect to the center of gravity of the pair) are $x_1 = -a/2$, $y_1 = 0$ and $x_2 = a/2$, $y_2 = 0$, respectively. In the y-state, we have $x_1 = 0$, $y_1 = -a/2$ and $x_2 = 0$, $y_2 = a/2$. From this we find operators of coordinates for both electrons:

$$x_1 = -x_2 = -\frac{a}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad y_1 = -y_2 = -\frac{a}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{30}$$

The operators of velocities are determined by the commutators

$$\dot{\mathbf{r}}_{1,2} = \frac{i}{\hbar} \left[H, \mathbf{r}_{1,2} \right]. \tag{31}$$

Simple calculation gives

$$\dot{x}_1 = -\dot{x}_2 = -\dot{y}_1 = \dot{y}_2 = -\frac{2at}{\hbar} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \equiv -\frac{2at}{\hbar}\sigma_2. \tag{32}$$

The operator of the pair magnetic moment which is directed along z-axis, is

$$\mu \equiv \mu_z = \frac{e}{2c} \sum_{1,2} (x\dot{y} - y\dot{x}) = -\frac{eta^2}{\hbar c}\sigma_2 \tag{33}$$

where e is the electron charge and c is the velocity of light.

In the presence of an external magnetic field $B \equiv B_z$, the Hamiltonian of the pair is

$$H = 4t\sigma_1 - \mu B. \tag{34}$$

The eigenvalues of energy are

$$E = \epsilon_0 \mp 4t \left[1 + \left(\frac{ea^2}{4\hbar c} B \right)^2 \right]^{1/2}. \tag{35}$$

In weak fields, the minimal energy is

$$E_{min} = \epsilon_0 - 4t - t\frac{e^2a^4}{8\hbar^2c^2} B^2. \tag{36}$$

The average magnetic moment of the pair is

$$\langle \mu \rangle = -\frac{\partial E_{min}}{\partial B} = \alpha B, \tag{37}$$

where

$$\alpha = \frac{e^2a^4}{4\hbar^2c^2} t = \frac{e^2a^2}{4mc^2} \tag{38}$$

is the pair paramagnetic polarizability.

We note that pairs with $\mathbf{k} = 0$ in the upper energy band (lower sign in (35)) are diamagnetic.

The pair contribution to the paramagnetic susceptibility of 3D sample is

$$\chi = \frac{e^2 a^2}{4mc^2} N^{(3)} \tag{39}$$

where $N^{(3)} = N(T)/L$ is 3D density of pairs and $N(T)$ is 2D density which is determined by formulas (16), (18), and (20). Here L is the distance between neighboring CuO_2 planes.

Generally, we have three competing contributions to the magnetic susceptibility: orbital paramagnetism of pairs considered above, Pauli spin susceptibility of single electrons (pairs are singlet), and Landau diamagnetism of single electrons and pairs. Spin susceptibility is isotropic. Orbital paramagnetism and Landau diamagnetism are both strongly anisotropic (magnetic moment is directed along z-axis independently of the direction of magnetic field) because of 2D character of single electrons and pairs. However, Landau diamagnetism, especially in 2D case, is very sensitive to inhomogeneities. For example, it is easily suppressed by a localization of charge carriers. Orbital paramagnetism is finite at zero velocity of a pair as a whole. So, it has to be much more stable against inhomogeneities. We hope that orbital paramagnetism can be experimentally separated from two other contributions to the susceptibility.

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